

# Coexistence of Non-Fermi Liquid and Fermi Liquid Self-Energies at All Dopings in Cuprates

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Non-Fermi liquid (NFL) state represents an ensemble of incoherent quantum fluids arising from the coupling between electrons and massless (critical) excitations, and is separated by phase boundary from the quasiparticle behavior in the Fermi-liquid (FL) theory. Here we show that such sharp distinction breaks down in cuprates, and that both NFL and FL states coexist in different momentum ( $k$ ) regions at all dopings. Their coexistence originates from the strong anisotropy in the many-body self-energy, arising from dispersive density-density fluctuations. The self-energy attains maxima (NFL-like) in the region where density degeneracy is optimum (antinodal region), while the nodal region remains FL-like at all dopings. We attribute the global NFL/FL behavior via the calculation of the resistivity-temperature exponent ( $n$ ). Surprisingly, we find that the entire Brillouin zone becomes neither fully incoherent, NFL-like even at optimal doping with  $n \sim 1$ , nor fully FL-like even at overdoping ( $n \sim 2$ ). As density degeneracy increases in different materials with increasing superconducting  $T_c$ ,  $n$  decreases; providing a microscopic explanation to this intriguing relationship. All results, including coexistence of NFL- and FL-self-energies in the  $k$ -space, and their doping, materials dependencies are compared with available experimental data, followed by definite predictions for future studies.

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## I. INTRODUCTION

Non-Fermi liquid (NFL) or strange metal phase is often observed to precede many correlated phases, such as antiferromagnetism, and unconventional superconductivity.<sup>1-3</sup> It is characterized by deviation from the well-defined Fermi-liquid (FL) predictions, such as the resistivity-temperature exponent ( $n$ ) being  $\sim 1$ , while  $n = 2$  is expected from the FL theory. Systematic studies in various superconducting families have also revealed that superconducting transition temperature ( $T_c$ ) increases as the exponent  $n$  decreases, i.e., as the system deviates farther from the FL behavior.<sup>1,4-6</sup> Therefore, NFL state is considered an important problem towards the understanding of unconventional superconductivity.

In the phase diagram, NFL state is often seen to arise near the boundary between an order phase and the FL state, where superconductivity is optimized.<sup>2,4-7</sup> Yet, considerable counter-examples are also present where a NFL phase is present without a quantum phase transition<sup>3,8-11</sup> or superconductivity.<sup>12</sup> Therefore, it has remained a ‘chicken-and-egg’ type problem whether a quantum critical point drives the NFL state or vice versa, and how they conspire into superconductivity.

To definitely answer this issue, one can approach the NFL state from the FL regime. The transition from the FL to NFL state is very adiabatic, i.e, the resistivity exponent  $n$  continuously changes from 2 (FL) to 1 or even below 1 in the NFL state at a given temperature. Theoretical models, relying on either critical fluctuations,<sup>2,13-16</sup> or marginal fluctuations,<sup>17</sup> or other quantum fields,<sup>18-24</sup> predict that when quantum fluctuations become gapless (critical), the low-energy excitation spectrum becomes linear in energy in the entire Brillouin zone (BZ), and the quasiparticle description fully breaks down. In such a case, the transport relaxation rate behaves as  $\tau^{-1} \propto (k_B T)$ , giving a linear resistivity exponent ( $n = 1$ ). On the other hand, the weak correlation in the FL regime gives a quadratic energy dependence of the excitations, and the cor-

responding low-energy quasiparticles produce  $n = 2$ . Model descriptions thus treat these regimes separately, and often unable to reconcile the adiabatic crossover between the FL to NFL states within a unified, self-consistent framework.<sup>20</sup>

Here we present a theory of the NFL phenomena arising from the *momentum* dependent self-energy due to canonical density-density fluctuations. The many-body self-energy is calculated based on the momentum-resolved density-fluctuation (MRDF) model within the fluctuation-exchange approximation.<sup>25-27</sup> The method is known to be appropriate for the intermediate coupling region where quantum fluctuations are of the order of the kinetic energy, stipulating a dynamically frustrated system. We apply the result in various cuprate materials.

We find that the dominant source of the NFL state stems from large degeneracy in the quasiparticle density. The NFL strength is incipiently controlled by the position of the DOS degeneracy from the Fermi level ( $\xi_F$ ) as well as its occupied momentum space volume (i.e. the amount of degeneracy) at a given condition. One of our key results is that even in the extreme NFL state where  $n \sim 1$  (near the optimal doping in cuprates), not all electronic states in the BZ become incoherent. Conversely, in the FL state (in overdoped region), not all quasiparticles are necessarily long-lived. This can be understood from the behavior of the  $k$ -dependent self-energy  $\Sigma''(\mathbf{k}, \omega) \propto |\omega|^{p_k}$ , allowing a  $k$ -dependent exponent  $p_k$ . We find that  $p_k$  strongly varies in the BZ: the high-density region (‘hot-spots’) governs  $p_k \sim 1$ , while the low-density region (‘cold-spots’) gives  $p_k \sim 2$ . This allows a coexistence and competition between the NFL and FL physics in the same system. The spectral weight transfer between the ‘hot-’ and ‘cold-spots’, caused by doping, temperature, and other parameters, manifests into an adiabatic transition between the FL and the NFL state. The results are applicable to a wider class of correlated materials in which large density of states is caused by van-Hove singularity (VHS), or Lifshitz points (as in pnictides), spin-orbit coupling (in heavy-fermions and

actinides) and leads to strong anisotropic self-energy effects.

We also make direct comparison with corresponding experiments. A recent angle-resolved photoemission spectroscopy (ARPES) experiment also observed a similar  $k$ -dependence in the electronic life-time in La-based cuprate.<sup>29</sup> It was found that the inverse of the quasiparticle lifetime changes from quadratic to linear as we move from nodal to the antinodal region, even in the overdoped sample where the transport data suggest a simple FL behavior. Again, angle-dependent magnetoresistance (ADMR) measurements on overdoped Tl-based cuprate also exhibited the similar behavior, in that the scattering rate becomes quadratic to linear-in- $T$  as we moves from the nodal to the antinodal region of the sample.<sup>30,31</sup>

The rest of the paper is organized as follows. In Sec. II, we discuss the MRDF model and the tight-binding dispersion. Momentum-dependent self-energy results and comparison with experiment is done in Sec. III. The overall FL/NFL behavior of a given system is characterized by the resistivity calculation and its doming dependence are discussed in Sec. IV. In Sec. V, we study the materials dependence of the resistivity-temperature exponent and its dependence with superconducting transition temperature is presented. Finally, we conclude in Sec. VI. The robustness of the results against the value of the Hubbard interaction  $U$  is demonstrated in the Appendix B.

## II. MRDF MODEL

Cuprate is a prototype of correlated superconducting family where the interplay between NFL, unconventional superconductivity, and various intertwined orders leads to a complex doping dependent phase diagram (see Fig. 1).<sup>32,33</sup> Yet, the band structure is rather straightforward with a single and strongly anisotropic band passing through the Fermi level. We consider a realistic band structure including upto fourth order tight-binding hoppings ( $t$ ,  $t'$ ,  $t''$ , and  $t'''$ ) as  $\xi_k = -2t(\cos k_x + \cos k_y) - 4t' \cos k_x \cos k_y - 2t''(\cos 2k_x + \cos 2k_y) - 4t''' \cos 2k_x \cos 2k_y - \xi_F$ . The second nearest neighbor hopping  $t'$  has a special importance in cuprates as it controls the flatness of the band near  $k = (\pi, 0)$  and its equivalent points. This generates paramount degeneracy in the DOSs at the VHS position. Interestingly, an earlier Density Functional Theory (DFT) calculation demonstrated that the optimal  $T_c$  in different cuprates scales almost linearly with the corresponding  $t'/t$  ratio.<sup>34</sup> It is also known that the energy of the VHS in a given system moves closer to the Fermi level with increasing doping, and crosses it in the vicinity of the optimal doping, see Fig. 1. These results give an important clue that the density fluctuation driven NFL is concentrated at the VHS region, while the other parts of the BZ continue to be FL-like. Their competition is controlled by chemical potential (doping) and  $t'$  (materials, pressure).

The density fluctuations dominate in the magnetic channel, giving paramagnon excitations in cuprates. These excitations are strongly dispersive, and present at all dopings.<sup>35</sup> The coupling between density fluctuations and electrons gives rise to a complex self-energy, which can be calculated in

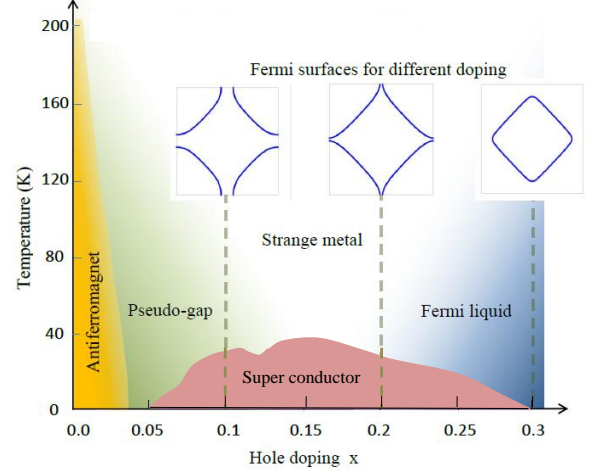


FIG. 1. (Color online) Schematic phase diagram of LSCO, showing the evolution of the Fermi surface across the NFL state and superconductivity. Around  $x \sim 0.2$ , the topological Fermi surface transition occurs where the VHS crosses  $\xi_F$ , and the corresponding resistivity exponent becomes also minimum.

a variety of numerical techniques.<sup>36</sup> Here we invoke a self-consistent momentum-resolved density fluctuation (MRDF) technique<sup>25–28</sup> which is suitable for the intermediate coupling regime where kinetic energy and dynamical correlations are comparable. The advantage of this technique is that it can efficiently calculate the full  $k$ -dependence of the self-energy. The self-energy in the fluctuation-exchange approximation is obtained as (see appendix C)

$$\Sigma_\nu(\mathbf{k}, \omega) = \frac{1}{N} \sum_{\mathbf{q}} \int_0^\infty \frac{d\varepsilon}{2\pi} \int_{-\infty}^\infty \frac{d\omega'}{2\pi} \Gamma(\mathbf{k}, \mathbf{q}) V_\nu(\mathbf{q}, \varepsilon) \times A(\mathbf{k} - \mathbf{q}, \omega') \left[ \frac{1 - f(\omega') + n(\varepsilon)}{\omega + i\delta - \omega' - \varepsilon} + \frac{f(\omega') + n(\varepsilon)}{\omega + i\delta - \omega' + \varepsilon} \right] \quad (1)$$

where  $f(\omega)$  and  $n(\varepsilon)$  are fermionic and bosonic distribution functions, respectively.  $N$  is the total number of lattice sites.  $A(\mathbf{k}, \omega) = -\text{Im}G(\mathbf{k}, \omega)/\pi$  and  $G(\mathbf{k}, \omega) = [\omega - \xi_k - \Sigma(\mathbf{k}, \omega)]^{-1}$  are the self-energy dressed spectral weight and Green's function, respectively. The vertex correction is  $\Gamma(\mathbf{k}, \mathbf{q}) = 1 - (\partial \Sigma'(\mathbf{k} - \mathbf{q}, \omega)/\partial \omega)_0$ .  $V_\nu(\mathbf{q}, \varepsilon)$  is the back-reaction potential of quasiparticle density fluctuation which is separated into the spin ( $\nu = 1$ ) and charge ( $\nu = 2$ ) density channels as

$$V_\nu(\mathbf{q}, \varepsilon) = \frac{\eta_\nu}{2} \text{Im} \left[ \frac{U^2 \chi(\mathbf{q}, \varepsilon)}{1 \mp U \chi(\mathbf{q}, \varepsilon)} \right], \quad (2)$$

where  $\eta_1 = 3$ , and  $\eta_2 = 1$ , and  $U$  is the onsite Hubbard interaction.  $\chi$  is the corresponding bare correlator (same for both spin and charge channels), evaluated self-consistently, as

$$\chi(\mathbf{q}, \varepsilon) = \frac{1}{N} \sum_{\mathbf{k}} \int \frac{d\omega_1}{2\pi} \int \frac{d\omega_2}{2\pi} A(\mathbf{k}, \omega_1) A(\mathbf{k} + \mathbf{q}, \omega_2) \times \frac{f(\omega_1) - f(\omega_2)}{\varepsilon + i\delta - \omega_2 + \omega_1}. \quad (3)$$

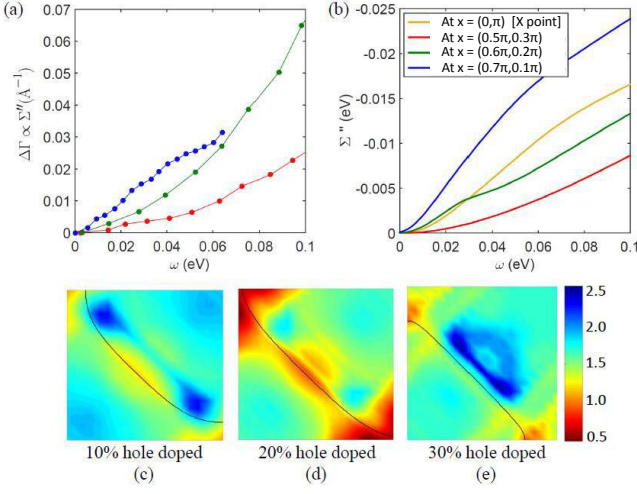


FIG. 2. (Color online)  $k$ -profile of  $\Sigma''$  for different dopings in LSCO. (a) Experimental data of  $\Sigma''(\omega)$  at three characteristic  $k$ -points in the overdoped sample (23% doping). The result clearly shows the transition from quadratic to linear  $\omega$ -dependence as we move from nodal to antinodal directions on the FS.<sup>29</sup> (b) Corresponding calculated  $\Sigma''(\omega)$  at different  $k$ -points. Same color (red, blue, green) represents same  $k$ -points in (a) and (b). (c-e) We show the self-energy exponent  $p_k$  in the entire first quadrant of the BZ in the underdoping, optimal doping, and the overdoped regions, respectively. Bottom-left corner is at the  $\Gamma$ -point, while the top-right corner is the  $(\pi, \pi)$ -point. The black line indicate the corresponding FS and the colorbar indicates the value of exponent  $p_k$ .

The tight-binding parameters and the Hubbard  $U$  for different materials are deduced from DFT calculations, and are listed in appendix A, and  $\xi_F$  is calculated self-consistently at each doping.

### III. SELF-ENERGY RESULTS

The real part of the self-energy  $\Sigma'(\mathbf{k}, \omega)$  renormalizes the band as  $Z_k \xi_k$ , where  $Z_k = (1 - \partial \Sigma'(\mathbf{k}, \omega) / \partial \omega)_0^{-1}$ . The corresponding spectral weight is determined by the combined effects of  $Z_k$  for  $\omega \rightarrow 0$ , and  $\Sigma''(\mathbf{k}, \omega)$  at finite energy. We fit  $\Sigma''(\mathbf{k}, \omega) = a_k |\omega|^{p_k}$  (where  $a_k$  is a proportionality constant).  $Z_k$  and  $p_k$  behave similarly (since  $\Sigma'$  and  $\Sigma''$  are connected to each other via Kramer's-Kronig relation): lower their values imply stronger the correlation strength at a given  $\mathbf{k}$ . In Fig. 2, we show the  $k$ - and doping dependence of  $\Sigma''$  and  $p_k$  for a representative material  $\text{La}_{2-x}\text{Sr}_x\text{CuO}_4$  (LSCO). The results are compared with the corresponding angle-resolved photoemission spectroscopy (ARPES) data.  $k$ -resolved values of the half-width half-maximum linewidth (defined as  $\Delta\gamma(k, \omega) = \gamma(\mathbf{k}, \omega) - \gamma(\mathbf{k}, 0) \propto -\Sigma''(\mathbf{k}, \omega)$ ) of the ARPES spectral weight show that the exponent  $p_k$  gradually decreases as one moves from the nodal region ( $p_k \sim 2$ ) to the antinodal one ( $p_k \sim 1$ ).<sup>29</sup> Our theoretical result, shown in Fig. 2(b), shows a similar behavior in that  $p_k \sim 2$  near the nodal region, which decreases to  $\sim 1$  as one reaches the antinodal region.

The full  $k$ -space profile for  $p_k$  is shown in Figs. 2(c-e) for

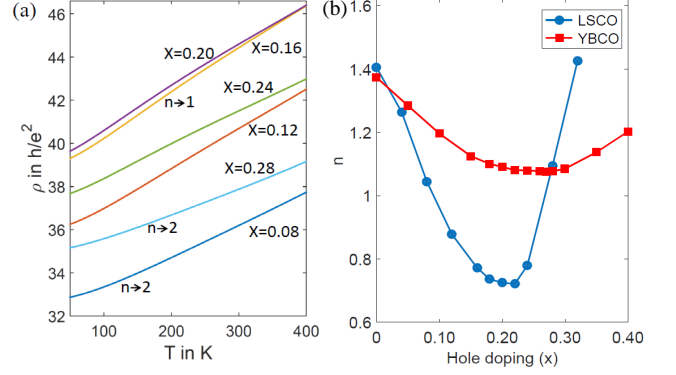


FIG. 3. (Color online) Resistivity is plotted as a function of temperature for different doping for LSCO. (Due to finite broadening of the Green's function at very low frequency  $\omega < 0.01\text{eV}$ , we cannot determine the exponent at very low-temperature.) The corresponding exponent of each curve is indicated in the adjacent label. (b) The resistivity-temperature exponent in the low- $T$  region is plotted as a function of dopings for two different materials. Both materials exhibit minimum in exponent near the optimal dopings where the corresponding VHS passes through the Fermi level.

three characteristic hole dopings for the same material (black line gives the corresponding non-interacting FS). The overall  $k$ -dependence of  $p_k$  remains similar at all dopings:  $p_k$  attains its minimum value around the antinodal region and maximum somewhere around the nodal region. In the underdoped region, where the VHS is well below  $\xi_F$ , we find that the overall  $p_k$  profile is less  $k$ -sensitive, and varies within the range of  $1.3 \lesssim p_k \lesssim 2.5$ . Near the optimal doping, where the VHS exactly crosses above  $\xi_F$ , we find that the  $k$ -dependence of  $p_k$  becomes strongest, and also  $p_k$  obtains its minimum value of  $\sim 0.5$  at the antinodal region. This is also the minimum possible value of  $p_k$  at all dopings and momenta for this material. In this region, we find that the resistivity-temperature exponent also attains its minimum value of  $\sim 0.7$  as shown in Fig. 3(b). Finally, as the VHS crosses above  $\varepsilon_F$ , again the value of  $p_k$  increases, indicating that the strength of dynamical correlation is maximum around the optimal doping where the Fermi surface degeneracy is highest.<sup>37</sup> Interestingly, in the overdoped region, where the resistivity data below shows an overall FL-behavior, the antinodal regions continue to show NFL self-energy behavior, in consistent with the ARPES data on LSCO at  $x = 0.23$ .<sup>29</sup>

As mentioned above, the momentum profile of  $p_k$  is similar to that of  $Z_k$ , and thus the spectral weight distribution on the Fermi surface also becomes characteristically the same. In what follows, the spectral weight at the antinodal region becomes minimum (where  $Z_k$  is maximum) and it gradually increases as one moves to the nodal region, giving a Fermi arc shape of the Fermi surface, a trademark feature of cuprate fermiology.<sup>38</sup>

#### IV. RESISTIVITY CALCULATIONS

When the  $k$ -dependence of the self-energy is neglected, a direct relation between the microscopic single-particle spectral properties (quantified by  $p$ ) and the macroscopic transport behavior ( $n = p$ ) can be established. However, as the system acquires strong anisotropy in  $p_k$ , it becomes less intuitive to deduce the overall correlation landscape of the system by the transport behavior. We compute the temperature dependence of the resistivity by including the full momentum and energy dependence of the self-energy. Within the linear response theory, the dc conductivity can be calculated from the current-current correlation function in the equivalent way as the density correlation is evaluated in Eq. (3), and we obtain:

$$\sigma_{xx} = \frac{e^2}{3\hbar^2} \frac{1}{N} \sum_{\mathbf{k}} v_x^2(\mathbf{k}) \int \frac{d\omega}{2\pi} A^2(\mathbf{k}, \omega) \left( -\frac{df(\omega)}{d\omega} \right), \quad (4)$$

where  $e$  and  $\hbar$  have the usual meanings, and  $v_i(\mathbf{k}) = -\partial G^{-1}(\mathbf{k}, 0)/\hbar \partial \mathbf{k}_i$  is the band velocity. Neglecting any anomalous term, we obtain resistivity as  $\rho = 1/\sigma$ . The results are presented in Fig. 3(a) for LSCO at different dopings. We find that the resistivity exponent becomes minimum near the optimal doping where the VHS crosses  $\xi_F$ , see Fig. 3(b). Here, the system acquires dominant NFL-behavior with  $n \sim 1$ . At the same doping, the self-energy exponent  $p_k$  in Fig. 2(d) not only obtains its minimum value ( $\min[p_k] \sim 0.5$ ), but also it occupies larger  $k$ -space area. However, the other parts of the BZ remains FL-like with  $p_k$  as large as  $\sim 2$ . Similarly, in both under- and overdopings, where  $n \rightarrow 2$ , the antinodal region continues to have  $p_k \sim 1$ . Finally, we repeat the calculation for the YBCO material as a function of doping, using the corresponding realistic tight-binding parameter set,<sup>25</sup> and the result is plotted in Fig. 3(b). We consistently find that  $n$  is minimum near its optimal doping as the corresponding VHS passes through  $\xi_F$ .

ADMR technique has the ability to probe the angle-variation of the resistivity by tilting the magnetic field with the sample orientation. This allows to effectively measure the scattering life-time  $1/\tau \propto \rho$  as a function of Fermi surface angle  $\theta = \tan^{-1}(k_y/k_x)$ . An earlier ADMR study on overdoped  $\text{Ti}_2\text{Ba}_2\text{CuO}_{6+x}$  found that  $1/\tau$  varies as  $T^2$  in the nodal region ( $\theta = 0$ ) and it gradually changes to  $T$  in the antinodal region ( $\theta = 45^\circ$ ).<sup>30,31</sup> This result is consistent with our finding of quasiparticle life-time variation shown in Fig. 2. Note that even the overall resistivity exponent is close to 2 in the overdoped region, however, its local variation reveals that both the single-particle life-time and scattering rate consistently remains incoherent in the antinodal region.

#### V. MATERIALS DEPENDENCE OF $n$ AND ITS CORRELATION WITH $T_c$

The celebrated paper by Pavarini *et al.*<sup>34</sup> pointed out an intriguing relationship between the  $t'/t$  ratio obtained in different materials with their  $T_c$ .  $t'/t$  triggers higher degeneracy in the DOS (see appendix B3), and hence it is natural to expect

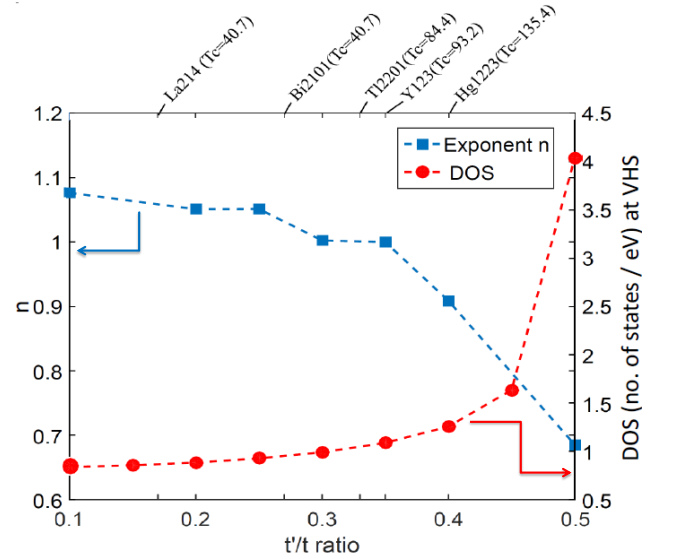


FIG. 4. (Color online) The resistivity exponent  $n$ , at the doping where the VHS passes through the Fermi level, is plotted for different values of  $t'/t$ , representing different cuprate materials.<sup>34</sup> This is the minimum value of  $n$  obtained across the doping range for a given  $t'/t$  since the DOS at  $E_F$  is maximum here (see the circle symbols for the DOS in the right-hand panel). At the top of the figure, we mention the corresponding cuprate materials with corresponding  $T_c$ , having different values of  $t'/t$  as obtained from the DFT calculation in Ref. 34. Chemical compositions of cuprate materials are:  $\text{La}_2\text{CuO}_4$  (La214),  $\text{Bi}_2\text{Sr}_2\text{CuO}_6$  (Bi2101),  $\text{Ti}_2\text{Ba}_2\text{CuO}_6$  (Ti2201),  $\text{YBa}_2\text{Cu}_3\text{O}_7$  (Y123),  $\text{HgBa}_2\text{Ca}_2\text{Cu}_3\text{O}_8$  (Hg1223).

that the strength of the NFL state would also increase. We calculate the resistivity exponent  $n$  for different values of  $t'/t$  by fixing the VHS at the  $\xi_F$ , and the result is plotted in Fig. 4. Indeed, we find that with increasing  $t'/t$ ,  $n$  decreases, that means, the system becomes more NFL like. With increasing  $t'/t$ , both the DOS at VHS increases and the bandwidth decreases (see appendix B3), and thus the NFL phenomena also increases. It is already known that the optimal  $T_c$  increases with increasing  $t'/t$ ,<sup>34</sup> and with decreasing  $n$ . Interestingly, it is also observed that as  $n$  decreases, the residual resistivity,  $\rho_0$  as  $T \rightarrow 0$ , also decreases, and  $T_c$  increases. This phenomena is consistently observed in various cuprates, pnictides and heavy-fermions.<sup>3</sup> Our results thus give the microscopic insight into this empirical observation.

#### VI. DISCUSSIONS AND CONCLUSIONS

Finally, we discuss various other phenomena in cuprates and their impact on our conclusions. The doping dependence of the dynamical correlation is different from that of the static correlation. The dynamical correlation, arising from the density fluctuation is determined by the strength of degeneracy (here VHS). It becomes dominant near the optimal doping where the VHS lies at  $\xi_F$ . On the other hand, static correlation is determined by the onsite Coulomb interaction ( $U$



in Eq. (2)) and it gives rise to a Mott insulator state at half-filling. While the static correlation decreases with doping, kinetic frustration increases and becomes maximum near the optimal doping at the VHS point. Kinetic frustration also introduces other competing phases such as antiferromagnetism, charge-density wave order, and other orders, and can modify the results in the underdoped region. Yet, without including any order parameter or quantum critical point, we get a good, quantitative agreement between the theory and experiment in the entire doping regime, suggesting that the dominant NFL physics stems from the DF fluctuations in these systems.

We have also studied all the results presented here for different values of  $U$ , and shown that the momentum profile of  $p_k$ , doping dependence of  $n$  etc. remain the same for different values of  $U$ , except that their overall strength decreases with decreasing  $U$ , i.e., the system moves towards FL-like as static correlation decreases. The FL state is recovered in the weak-coupling region (see appendix B).

The important message of our result is that for strongly anisotropic materials where the dynamical fluctuations have significant momentum dependence, the resistivity-temperature exponent is not a robust measure of the full correlation spectrum of the underlying quasiparticle states. We found that even in the underdoped and overdoped regions, where resistivity exponent  $n \rightarrow 2$ , there are considerable amount of NFL-like incoherent states lying in the antinodal regions and vice versa. Similarly, in the extreme NFL region near the optimal doping regime (determined by  $n \sim 1$ ), the nodal quasiparticles continue to behave FL-like (with  $\Sigma'' \propto |\omega|^2$ ). Both as a function of temperature and doping (and other tunings), the spectral weight is transferred between the NFL and FL regions and the system adiabatically transforms from a dominant NFL to a FL-like state, as seen in experiments. Our work suggests that the microscopic and macroscopic landscapes of the NFL behavior can be characteristically different and that a direct correspondence between  $k$ -resolved spectroscopy (such as ARPES, and quasiparticle interference (QPI) pattern) and the transport, and thermodynamical properties are necessary to deduce the global and local NFL behavior of a given system.

#### Appendix A: Tight-binding parameters

Material	$t$	$t'$	$t''$	$t'''$	$U$	Reference
LSCO	0.4195	-0.0375	0.018	0.034	1.6	39
YBCO	0.35	-0.06	0.035	-0.005	1.9	40

TABLE I. Full tight binding parameters for different materials. All energies are given in eV.

#### Appendix B: $U$ Dependence of various results

All results and conclusions presented above are obtained for material specific values of the Hubbard  $U$ . In the Appendix, we investigate them for different values of  $U$  and establish their robustness. The following results also demonstrate the distinction between the doping dependence of the static correlation ( $U$ ) and the dynamical correlation ( $V(\omega)$  in Eq. 2).

##### 1. NFL to FL transition with decreasing $U$

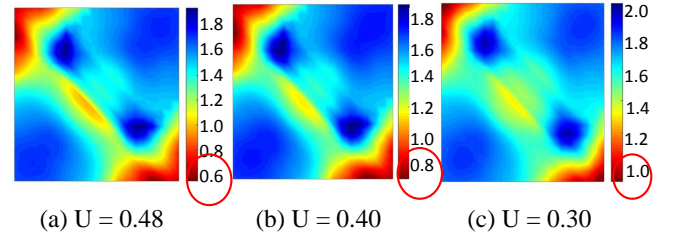


FIG. 5. (Color online) Plots of the self-energy power  $p_k$  (defined in the main text as  $\Sigma''(\mathbf{k}, \omega) \propto |\omega|^{p_k}$ ) for three different values of  $U$  for LSCO. In all three cases, we notice that the overall momentum profile of  $p_k$  remains the same, as we expect, since the momentum dependence is determined by the DOS ‘hot-spots’. The overall range of  $p_k$  (seen in the adjacent colorbars) however increases with decreasing  $U$ , which means the system moves towards the FL region at fixed doping as  $U$  decreases.

Keeping all other parameters the same, we expect that the system would tend to transform from NFL to FL like as we decrease the values of  $U$ . This is precisely what we observe in Fig. 5 where we plot the momentum profile of  $p_k$  at a fixed doping of  $x = 0.20$  for LSCO for three different values of  $U$ . In all three cases, the momentum profile remains very much the same, as we expect, since the momentum dependence is governed by the band structure anisotropy and spectral density ‘hot-spots’. We notice a characteristic change in the overall range of  $p_k$  (as highlighted by red circles in the adjacent colorbars). We find that both the minimum and the maximum values of  $p_k$  increases with decreasing  $U$ . In addition we also notice that the  $k$ -space area of the NFL region ( $p_k \sim 1$ ) also decreases with decreasing  $U$ , reflecting that the system moves towards FL as correlation weakens. The result is confirmed by the resistivity exponent calculation as presented in Fig. ref-figB2.

##### 2. Same phase diagram with different values of $U$

We obtain the same conclusion in the resistivity-temperature exponent  $n$ , calculated with the same parameter sets as in Fig. 5. We find that the overall doping dependence

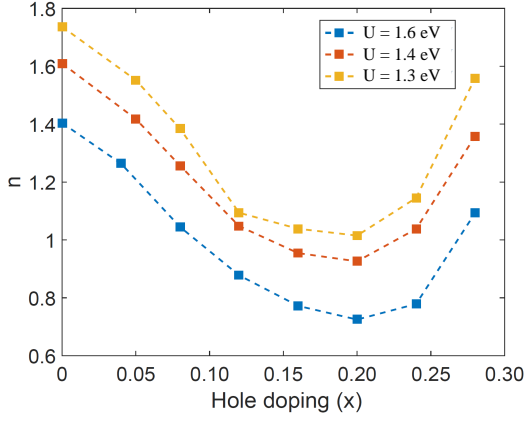


FIG. 6. (Color online) The resistivity exponent  $n$  is plotted as a function of doping for the same three values of  $U$  as in Fig. SI for LSCO.

of  $n$  is similar for all three values of  $U$ : it obtains the minimum value near the optimal doping where the VHS passes through the Fermi level, irrespective of the values of  $U$ . However, the overall value of  $n$  increases with decreasing  $U$  as the system moves towards the FL like with lowering its correlation strength.

### 3. Robustness of the $t'/t$ vs. $n$ plot for different $U$

Finally we study the evolution of the  $t'/t$  vs.  $n$  plot for different values of  $U$  in Fig. 7. We have learned in the main text that  $n$  decreases as the  $t'/t$  ratio increases, keeping the corresponding VHS fixed at the Fermi level for all cases. This is because the DOS at the VHS increases with increasing  $t'/t$  and the bandwidth simultaneously decreases. Therefore, the system becomes more NFL-like as  $t'/t$  increases. This conclusion remains intact as we tune the values of  $U$ . For different values of  $U$ , the general trend in  $n$  with  $t'/t$  remains the same, however the overall range of  $n$  increases with decreasing  $U$  as we also found in Figs. 5 and 6 before.

### Appendix C: Self-consistent susceptibilities and self-energy calculations

We start with the standard definition of spin/charge susceptibility<sup>42,43</sup> which is given by

$$\chi^{ij}(\mathbf{q}, \tau) = \frac{1}{N} \langle T_\tau \Pi^i(\mathbf{q}, \tau) \Pi^j(-\mathbf{q}, 0) \rangle, \quad (\text{C1})$$

where  $\Pi^i(\mathbf{q}, \tau)$  denotes the spin/charge density where indices  $i, j$  denote different components (for example  $x, y, z$  components) in case of spin susceptibility. Charge and spin densities

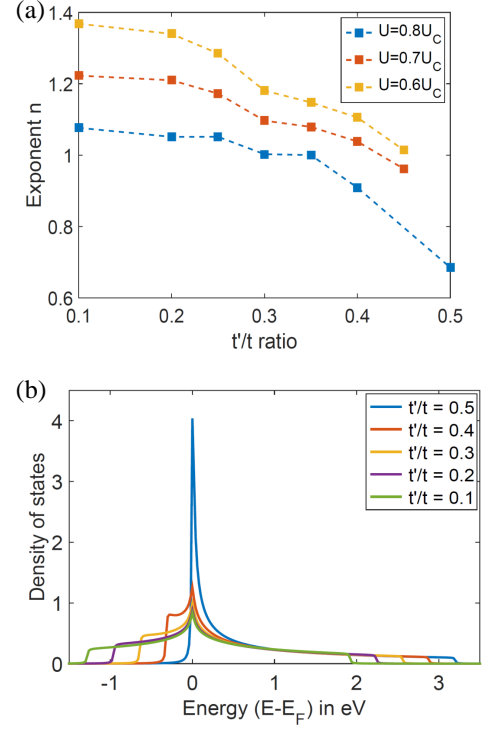


FIG. 7. (Color online) (a) Plots of  $t'/t$  vs.  $n$  for different values of  $U$ . As expected, the exponent  $n$  decreases with increasing  $U$ , but for all values of  $U$ , the  $t'/t$  dependence on  $n$  is maintained. (b) Density of states (DOS) is shown as a function of energy for different values of the  $t'/t$  ratio. Note that the DOS at the VHS gradually increases with increasing  $t'/t$  ratio, as the flatness of the band increases at the antinodal point. The Fermi level for all cases is fixed at the VHS.

$(\Pi^i(\mathbf{q}, \tau))$  are given in the second quantized notation as

$$\rho_{\mathbf{q}}(\tau) = \sum_{\mathbf{k}, \sigma} c_{\mathbf{k}+\mathbf{q}, \sigma}^\dagger(\tau) c_{\mathbf{k}, \sigma}(\tau), \quad (\text{C2})$$

$$S_{\mathbf{q}}^i(\tau) = \sum_{\mathbf{k}, \alpha, \beta} c_{\mathbf{k}+\mathbf{q}, \alpha}^\dagger(\tau) \sigma_{\alpha\beta}^i c_{\mathbf{k}, \beta}(\tau), \quad (\text{C3})$$

where  $\sigma^i$ s are the Pauli spin matrices in 2D.  $c_{\mathbf{k}, \sigma}^\dagger(\tau)$  is the dressed quasi-particle creation operator (sometimes called Dyson orbitals) at Bloch momentum  $\mathbf{k}$  and spin  $\sigma$ . Since the ground state is spinless, both transverse and longitudinal spin-densities, as well as the charge density term yields the same bare susceptibility. In general, we can write Eq. (C1) as

$$\chi(\mathbf{q}, \tau) = \frac{1}{N} \sum_{\mathbf{k}, \mathbf{k}', \sigma, \sigma', \sigma'', \sigma'''} \langle T_\tau c_{\mathbf{k}+\mathbf{q}, \sigma}^\dagger(\tau) c_{\mathbf{k}, \sigma'}(\tau) c_{\mathbf{k}'-\mathbf{q}, \sigma''}^\dagger(0) c_{\mathbf{k}', \sigma'''}(0) \rangle \quad (\text{C4})$$

where the momentum conservation is imposed. We can decompose the four-field terms into bi-linear terms within Wick's theorem, and allow the spin-conservation condition for

the ground state. Then we obtain,

$$\begin{aligned}\chi(\mathbf{q}, \tau) &= \frac{1}{N} \sum_{\mathbf{k}, \mathbf{k}', \sigma, \sigma', \sigma'', \sigma'''} \langle T_\tau c_{\mathbf{k}, \sigma}(\tau) c_{\mathbf{k}' - \mathbf{q}, \sigma'}^\dagger(0) \delta_{\sigma \sigma'''} \rangle \\ &\quad \times \langle T_\tau c_{\mathbf{k}', \sigma'}(0) c_{\mathbf{k} + \mathbf{q}, \sigma}^\dagger(\tau) \delta_{\sigma' \sigma''} \rangle, \\ &= \frac{1}{N} \sum_{\mathbf{k}, \sigma \sigma'} G_\sigma(\mathbf{k}, \tau) G_{\sigma'}(\mathbf{k} + \mathbf{q}, -\tau),\end{aligned}\quad (\text{C5})$$

where we have identified the terms in the brackets as self-energy dressed Green's functions such as

$$\begin{aligned}\langle T_\tau c_{\mathbf{k}, \sigma}(\tau) c_{\mathbf{k}' - \mathbf{q}, \sigma'}^\dagger(0) \rangle \\ = G_{\sigma \sigma'}(\mathbf{k}, \mathbf{k}' - \mathbf{q}, \tau) \delta_{\mathbf{k}, \mathbf{k}' - \mathbf{q}} \delta_{\sigma, \sigma'}\end{aligned}\quad (\text{C6})$$

$$\begin{aligned}\langle T_\tau c_{\mathbf{k}', \sigma'}(0) c_{\mathbf{k} + \mathbf{q}, \sigma}^\dagger(\tau) \rangle \\ = G_{\sigma' \sigma}(\mathbf{k}', \mathbf{k} + \mathbf{q}, -\tau) \delta_{\mathbf{k}', \mathbf{k} + \mathbf{q}} \delta_{\sigma', \sigma}.\end{aligned}\quad (\text{C7})$$

The Fourier transform of Green's function is defined as

$$G(\mathbf{k}, \tau) = \frac{1}{\beta} \sum_{\omega_n} e^{-i\omega_n \tau} G(\mathbf{k}, i\omega_n) \quad (\text{C8})$$

and that of the susceptibility as

$$\chi(\mathbf{q}, i\epsilon_m) = \frac{1}{N} \int_0^\beta \chi(\mathbf{q}, \tau) e^{i\epsilon_m \tau} d\tau. \quad (\text{C9})$$

Here  $i\omega_n$  and  $i\epsilon_m$  are the fermionic and bosonic Matsubara frequencies, respectively. Finally, we get

$$\begin{aligned}\chi(\mathbf{q}, i\epsilon_m) \\ = \frac{1}{N\beta^2} \sum_{\mathbf{k}, n, n'} \int_0^\beta e^{(-i\omega_n + i\omega_{n'} + i\epsilon_m)\tau} G(\mathbf{k}, i\omega_n) G(\mathbf{k} + \mathbf{q}, i\omega_{n'}) d\tau, \text{Im}\{W_\nu(\mathbf{q}, \epsilon)\}. \\ = \frac{1}{N\beta} \sum_{\mathbf{k}, i\omega_n} G(\mathbf{k}, i\omega_n) G(\mathbf{k} + \mathbf{q}, i\omega_n - i\epsilon_m).\end{aligned}\quad (\text{C10})$$

From here onwards we drop the index  $\sigma$  and assume an implied sum over  $\sigma$  index. It is not easy to perform the Matsubara frequency summation using self-energy dressed Green's function. So we use its spectral representation as

$$G(\mathbf{k}, i\omega_n) = \int_{-\infty}^{\infty} \frac{d\omega_1}{2\pi} \frac{A(\mathbf{k}, \omega_1)}{i\omega_n - \omega_1}, \quad (\text{C11})$$

where  $A$  is the corresponding spectral weight defined as  $A(\mathbf{k}, \omega) = -\text{Im}G(\mathbf{k}, \omega)/\pi$ , where  $G(\mathbf{k}, \omega)$  is obtained by taking the analytical continuation to the real frequency  $i\omega_n =$

$\omega + i\delta$ , with  $\delta$  being infinitesimal broadening. So the susceptibility expression becomes

$$\begin{aligned}\chi(\mathbf{q}, i\epsilon_n) &= \frac{1}{N} \sum_{\mathbf{k}} \int_{-\infty}^{\infty} \int_{-\infty}^{\infty} \frac{d\omega_1}{2\pi} \frac{d\omega_2}{2\pi} A(\mathbf{k}, \omega_1) A(\mathbf{k} + \mathbf{q}, \omega_2) \\ &\quad \times \left( \frac{1}{\beta} \sum_{p_n} \frac{1}{i\epsilon_n - \omega_1} \frac{1}{i\omega_n - i\omega_n - \omega_2} \right).\end{aligned}\quad (\text{C12})$$

The term in the bracket can be evaluate by Matsubara technique<sup>42</sup> and we arrive at the expression

$$\begin{aligned}\chi(\mathbf{q}, i\omega_n) &= \frac{1}{N} \sum_{\mathbf{k}} \int_{-\infty}^{\infty} \int_{-\infty}^{\infty} \frac{d\omega_1}{2\pi} \frac{d\omega_2}{2\pi} A(\mathbf{k}, \omega_1) \\ &\quad \times A(\mathbf{k} + \mathbf{q}, \omega_2) \frac{f(\omega_1) - f(\omega_2)}{i\omega_n - \omega_2 + \omega_1},\end{aligned}\quad (\text{C13})$$

where  $f(\omega)$  denotes the Fermi distribution function. The computation of the susceptibility is done using analytical continuation to the real frequency as discussed before.

Next we calculate the self energy starting from GW approximation<sup>44-46</sup> which is given by

$$\begin{aligned}\Sigma_\nu(\mathbf{k}, i\omega_n) &= -\frac{1}{N\beta} \sum_{\mathbf{q}, m} G(\mathbf{k} - \mathbf{q}, i\omega_n - i\epsilon_m) \\ &\quad \times W_\nu(\mathbf{q}, i\epsilon_m) \Gamma(\mathbf{k}, \mathbf{q}),\end{aligned}\quad (\text{C14})$$

where  $\Gamma(\mathbf{k}, \mathbf{q})$  is the vertex correction discussed in the main text.  $W$  is the fluctuation-exchange potential which we obtain within the random-phase approximation as

$$W_\nu(\mathbf{q}, i\epsilon_m) = \frac{\eta_\nu}{2} \frac{U^2 \chi(\mathbf{q}, i\epsilon_m)}{1 \pm U \chi(\mathbf{q}, i\epsilon_m)}, \quad (\text{C15})$$

where  $\eta = 3$  and  $1$  for spin ( $\nu = 1$ ) and charge ( $\nu = 2$ ) density fluctuations. Again, to aid the Matsubara frequency summation, we use the spectral representation of  $W$  as

$$W_\nu(\mathbf{q}, i\epsilon_m) = \int_{-\infty}^{\infty} \frac{d\epsilon'}{2\pi} \frac{\text{Im}\{W_\nu(\mathbf{q}, \epsilon')\}}{i\epsilon_m - \epsilon'}. \quad (\text{C16})$$

We denote the fluctuation-exchange potential as  $V_\nu(\mathbf{q}, \epsilon) = \text{Im}\{W_\nu(\mathbf{q}, \epsilon)\}$ . Therefore, using Eqs. (C14) and (C16), we get

$$\begin{aligned}\Sigma_\nu(\mathbf{k}, i\omega_n) \\ = -\frac{1}{N} \sum_{\mathbf{q}} \int_{-\infty}^{\infty} \frac{d\epsilon}{2\pi} \int_{-\infty}^{\infty} \frac{d\omega'}{2\pi} A(\mathbf{k} - \mathbf{q}, \omega') V_\nu(\mathbf{q}, \epsilon) \\ \times \Gamma(\mathbf{k}, \mathbf{q}) \left( \frac{1}{\beta} \sum_{\epsilon_m} \frac{1}{i\omega_n - i\epsilon_m - \omega'} \frac{1}{i\epsilon_m - \epsilon} \right) \\ = \frac{1}{N} \sum_{\mathbf{q}} \int_{-\infty}^{\infty} \frac{d\epsilon}{2\pi} \int_{-\infty}^{\infty} \frac{d\omega'}{2\pi} A(\mathbf{k} - \mathbf{q}, \omega') V_\nu(\mathbf{q}, \epsilon) \\ \times \Gamma(\mathbf{k}, \mathbf{q}) \frac{f(-\omega') + n(\epsilon)}{i\omega_n - \omega' - \epsilon},\end{aligned}\quad (\text{C17})$$

$$\begin{aligned}= \frac{1}{N} \sum_{\mathbf{q}} \int_{-\infty}^{\infty} \frac{d\epsilon}{2\pi} \int_{-\infty}^{\infty} \frac{d\omega'}{2\pi} A(\mathbf{k} - \mathbf{q}, \omega') V_\nu(\mathbf{q}, \epsilon) \\ \times \Gamma(\mathbf{k}, \mathbf{q}) \left[ \frac{1 - f(\omega') + n(\epsilon)}{i\omega_n - \omega' - \epsilon} + \frac{f(\omega') + n(\epsilon)}{i\omega_n - \omega' + \epsilon} \right]\end{aligned}\quad (\text{C18})$$

All other symbols were defined in the main text.

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- <sup>37</sup> Fermi surface degeneracy here does not refer to Fermi surface nesting, rather indicate that the degeneracy of the band is highest on the largest parts of the Fermi surface.
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